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Flow and Geomechanics in Fractured Black Shale

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Narrative Progress Report

This project aims to advance our capabilities to model the dynamic behavior of both fluids and rocks in fractured black shale formations. In this period, we advanced in three key areas: 1) characterizing fluid behavior, particularly sorption, in nano-porous materials, 2) characterizing the effective permeabilities and fluid migration histories of fractured shales, and 3) the modeling of coupled multiphase compositional fluid flow and geomechanical responses. Further details are provided below.

Sorption in Nanoporous Shales

In conventional rocks, the initial amount of fluids in place can be determined readily by multiplying a reservoir volume with its (effective/average) porosity; and fluid flow and transport are governed by well understood driving forces, e.g. through Darcy's law, Fickian diffusion, gravity, and capillary imbibition/drainage. In unconventional tight rocks, such as black shales, the situation is far more complex. *Bulk* gas may only be a minority component ($< 50\%$) of the total gas-in-place (GIP), with the majority of gas *adsorbed* onto the exceedingly large specific surface area (SSA) of very small pores (with values of SSA of the order of 10 m^2/g), and another significant fraction of gas *dissolved* inside the organic matter, such as kerogen. The transport processes in such nano-porous materials are also still poorly understood, and involves the desorption of gas as one of the processes required to produce significant amounts of gas.

Last year, we reported on PhD student Fengyang Xiong's efforts to characterize the pore size distribution and SSA of a range of shale samples and correlate those to mineralogy, organic matter, and maturity [2]. This year, Xiong has shifted his focus to a detailed study of the associated sorption behavior. In a first paper [1], he performed on-site canister desorption tests on a large number (33) of full-sized shale cores, which measure the volumes of gas emitted from the cores as soon as they are drilled and lifted to the surface. Desorption was measured both at the reservoir temperature and an elevated temperature of 95°C, showing a tight correlation between the cumulative volumes emitted at both temperatures. Considering the factors controlling this emission behavior, organic chemistry and X-ray diffraction measurements were used to establish relationships between the gas content and rock composition, showing that the total organic carbon (TOC) content is the main predictor of the desorption behavior in these large and heterogeneous cores (Fig. 1).

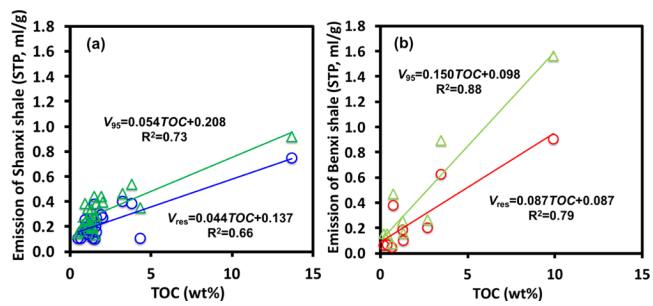

Figure 1: Correlation between emitted gas and TOC in Shanxi (a) and Benxi shales (b). Circles for reservoir temperature and triangles for 95 °C. (from: [1]).

Since then, Xiong has moved on to more controlled lab experiments measuring high pressure methane adsorption/desorption isotherms. These measurements are challenging and require sensitive instruments (e.g., a gravimetric Rubotherm) that are not widely available. After unsuccessfully trying to perform the experiments at OSU and his prior institution in Beijing, he was finally able to complete this work during a three month visit to the Oak Ridge National Lab facilities this past Summer. Excess sorption isotherms were measured for multiple samples of different TOC and mineral composition, and at three different temperatures (Fig. 2). Our key focus was on how to correct these *excess* isotherms to *absolute* sorption, which is the quantity of interest in estimating GIP. This correction depends on the density of the adsorption layer, which is not known. Prior work has assumed constant values, which are unphysical and lead to unreasonable GIP estimates. Xiong has proposed a novel method of estimating the *pressure dependent* density in the adsorption layer, which should signifi-

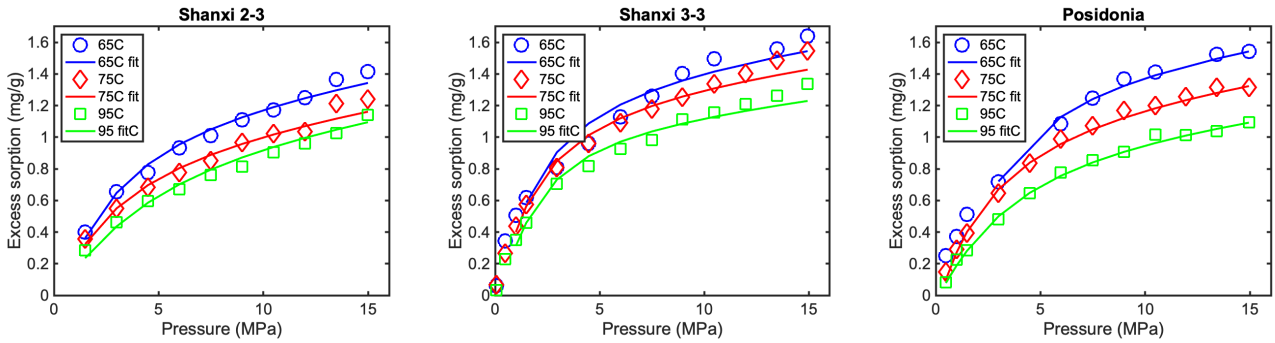

Figure 2: Excess sorption isotherms for 3 samples at 3 temperatures, fitted by Ono-Kondo model.

cantly improve our estimates of absolute adsorption in shale samples, and thus our estimates of total GIP (manuscript in in review). He has a number of additional papers in preparation that will make significant contributions to our understanding of fluid behavior in nanoporous shales.

Characterization of Natural Fractures in Shale Formations

A second PhD student, William Eymold, had intended to complete the main modeling component of this proposal in coupling our in-house reservoir simulator to another code for geomechanics, but instead decided to pursue a different direction in his PhD research that is still closely related to the project. Specifically, he is using a novel noble gas geochemistry technique on shale samples to determine the effective (natural) fracture intensity and orientations, as well as past fluid migration (as a proxy for fracture conductivity) in shale formations. This work is intended to provide us with the necessary field data to constrain future modeling of field-scale shale formations.

Coupled Multiphase Fluid Flow and Geomechanics

Because of the aforementioned, simulator development has been delayed and a no-cost extension was granted. A promising new student, Derrick James, has joined our team to complete this work. James recently graduated in Physics and Astronomy and has considerable prior programming experience. In June, we both participated in the 'coding bootcamp' Crustal Deformation Modeling Workshop at Colorado School of Mines related to the open source code *pylith*, which we intend to adopt for our geomechanics modeling, and established ties to their development team. This September, I also visited the Petroleum Engineering department at the University of Southern California to establish collaboration with a colleague who has similarly coupled *pylith* to another legacy reservoir simulator (for different types of applications). In addition, we have completed a new theoretical framework required for coupled poromechanics involving compressible, multiphase, and multicomponent compositional flow (manuscript in prep). Together, this lays the foundation to successfully complete our remaining project objectives going forward.

Summary of Support and Outcomes

The support provided by the ACS PRF has tremendously helped the career of 4 ambitious graduate students as well as my own. The first student on this project (Amooie) has already moved on to a postdoc at MIT and the second (Xiong) is planning to graduate soon and also pursue an academic career. All students involved have published in high-quality journals, presented their work at numerous conferences, and attracted additional external funding ($\sim \$50,000$) for their research. My own recent promotion to tenure would not have been possible without their hard work and financial support from this program.

References

[1] Fengyang Xiong, Zhenxue Jiang, Hexin Huang, Ming Wen, and Joachim Moortgat. Mineralogy and Gas Content of Upper Paleozoic Shanxi and Benxi Shale Formations in the Ordos Basin. *Energy & Fuels*, 33(2):1061–1068, 2019.

[2] Fengyang Xiong, Zhenxue Jiang, Peng Li, Xiangzeng Wang, He Bi, Yirun Li, Ziyuan Wang, Mohammad Amin Amooie, Mohamad Reza Soltanian, and Joachim Moortgat. Pore structure of transitional shales in the Ordos Basin, NW China: Effects of composition on gas storage capacity. *Fuel*, 206:504–515, 2017.